

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011024\
 Data File : VV033566.D
 Acq On : 10 Jan 2024 17:30
 Operator : SY/MD
 Sample : P1016-04 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCMH4

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
 Title : VOC Analysis

Signal : TIC: VV033566.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.278	68	74	90	rBV	186667	196789	15.27%	1.878%
2	1.532	146	153	172	rVB	142492	176728	13.71%	1.686%
3	2.060	309	317	329	rBV	288046	410053	31.82%	3.913%
4	2.449	429	438	449	rBV3	5960	10171	0.79%	0.097%
5	3.063	626	629	630	rBV2	461	265	0.02%	0.003%
6	3.105	635	642	666	rVV3	5977	14448	1.12%	0.138%
7	3.243	683	685	688	rBV4	399	166	0.01%	0.002%
8	3.404	733	735	738	rBV3	379	194	0.02%	0.002%
9	3.452	748	750	752	rBV2	221	111	0.01%	0.001%
10	3.526	771	773	775	rBV3	550	280	0.02%	0.003%
11	3.561	780	784	788	rBV6	490	424	0.03%	0.004%
12	3.641	806	809	811	rBV	274	168	0.01%	0.002%
13	3.670	814	818	821	rVV5	397	300	0.02%	0.003%
14	3.783	845	853	901	rBV	89596	252659	19.60%	2.411%
15	4.249	984	998	1028	rVB	190701	484202	37.57%	4.620%
16	4.567	1094	1097	1101	rBV5	600	617	0.05%	0.006%
17	4.680	1129	1132	1134	rBV2	753	477	0.04%	0.005%
18	4.719	1141	1144	1145	rBV3	340	161	0.01%	0.002%
19	4.789	1164	1166	1167	rBV	282	105	0.01%	0.001%
20	4.873	1187	1192	1195	rBV5	387	309	0.02%	0.003%
21	4.892	1195	1198	1199	rBV3	620	308	0.02%	0.003%
22	4.957	1202	1218	1247	rBV2	484843	1288828	100.00%	12.299%
23	5.535	1386	1398	1426	rBV	404214	831383	64.51%	7.933%
24	5.908	1512	1514	1516	rBV3	355	175	0.01%	0.002%
25	5.989	1526	1539	1569	rBV	284960	593151	46.02%	5.660%
26	6.394	1658	1665	1701	rBV	97639	196428	15.24%	1.874%
27	6.831	1799	1801	1806	rVB5	355	255	0.02%	0.002%
28	6.854	1806	1808	1810	rBV2	515	296	0.02%	0.003%
29	6.915	1816	1827	1853	rBV	165486	314920	24.43%	3.005%
30	7.124	1883	1892	1903	rBV	24083	41392	3.21%	0.395%
31	7.243	1918	1929	1966	rBV	577450	1035600	80.35%	9.882%
32	7.555	2017	2026	2050	rBV	139429	252398	19.58%	2.408%
33	7.863	2111	2122	2135	rBV	35882	62666	4.86%	0.598%
34	8.024	2163	2172	2198	rBV	330565	609231	47.27%	5.814%
35	8.249	2235	2242	2265	rVB	27139	51582	4.00%	0.492%
36	8.538	2329	2332	2334	rBV3	630	436	0.03%	0.004%

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Integrator: RTE

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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 Title : VOC Analysis

37	8.619	2347	2357	2379	rBV	101283	165816	12.87%	1.582%
38	8.786	2397	2409	2441	rBV	604670	1011313	78.47%	9.650%
39	9.210	2540	2541	2544	rVB2	357	185	0.01%	0.002%
40	9.243	2547	2551	2558	rBV5	633	788	0.06%	0.008%
41	9.271	2558	2560	2562	rVB2	297	64	0.00%	0.001%
42	9.288	2562	2565	2569	rBV5	482	466	0.04%	0.004%
43	9.349	2581	2584	2589	rBV5	587	551	0.04%	0.005%
44	9.458	2616	2618	2619	rBV	276	103	0.01%	0.001%
45	9.497	2619	2630	2640	rBV3	5833	11315	0.88%	0.108%
46	9.651	2676	2678	2680	rBV2	326	172	0.01%	0.002%
47	9.699	2690	2693	2697	rVB4	558	420	0.03%	0.004%
48	9.728	2697	2702	2704	rBV4	531	497	0.04%	0.005%
49	9.776	2713	2717	2719	rBV3	389	266	0.02%	0.003%
50	9.796	2719	2723	2725	rBV3	379	290	0.02%	0.003%
51	9.882	2746	2750	2753	rBV4	514	442	0.03%	0.004%
52	9.915	2757	2760	2761	rBV2	255	117	0.01%	0.001%
53	9.940	2766	2768	2771	rVB3	364	179	0.01%	0.002%
54	9.966	2771	2776	2780	rBV6	640	696	0.05%	0.007%
55	9.992	2782	2784	2786	rBV2	476	275	0.02%	0.003%
56	10.040	2794	2799	2805	rBV3	460	583	0.05%	0.006%
57	10.075	2805	2810	2812	rBV2	482	376	0.03%	0.004%
58	10.152	2823	2834	2856	rBV	350063	552549	42.87%	5.273%
59	10.577	2964	2966	2970	rBV3	286	177	0.01%	0.002%
60	10.599	2971	2973	2980	rVB5	550	502	0.04%	0.005%
61	10.699	3002	3004	3008	rBV4	438	276	0.02%	0.003%
62	10.728	3008	3013	3014	rBV4	554	519	0.04%	0.005%
63	10.818	3036	3041	3043	rBV4	605	385	0.03%	0.004%
64	10.863	3049	3055	3058	rBV3	620	713	0.06%	0.007%
65	10.924	3071	3074	3078	rVB4	501	327	0.03%	0.003%
66	11.078	3119	3122	3123	rVB	239	108	0.01%	0.001%
67	11.088	3123	3125	3131	rVB3	311	220	0.02%	0.002%
68	11.111	3131	3132	3134	rVB	220	67	0.01%	0.001%
69	11.133	3135	3139	3143	rBV6	1076	627	0.05%	0.006%
70	11.185	3143	3155	3179	rBV	624087	978057	75.89%	9.333%
71	11.464	3240	3242	3243	rBV2	261	134	0.01%	0.001%
72	11.477	3244	3246	3250	rVV2	511	354	0.03%	0.003%
73	11.519	3254	3259	3260	rBV4	587	382	0.03%	0.004%
74	11.561	3260	3272	3294	rBV	571597	906385	70.33%	8.649%
75	11.757	3330	3333	3337	rVB4	647	408	0.03%	0.004%
76	11.776	3337	3339	3340	rBV2	285	113	0.01%	0.001%

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 Title : VOC Analysis

77	11.847	3358	3361	3364	rBV3	385	234	0.02%	0.002%
78	11.908	3376	3380	3382	rBV3	642	434	0.03%	0.004%
79	12.078	3430	3433	3435	rVB4	426	238	0.02%	0.002%
80	12.217	3472	3476	3479	rBV3	568	305	0.02%	0.003%
81	12.275	3492	3494	3497	rBV3	435	214	0.02%	0.002%
82	12.345	3512	3516	3517	rBV3	655	454	0.04%	0.004%
83	12.474	3554	3556	3557	rBV	354	153	0.01%	0.001%
84	12.516	3567	3569	3571	rBV	326	100	0.01%	0.001%
85	12.754	3640	3643	3644	rVB2	395	184	0.01%	0.002%
86	12.770	3644	3648	3650	rBV4	411	293	0.02%	0.003%
87	13.104	3750	3752	3753	rBV	481	193	0.01%	0.002%
88	13.303	3812	3814	3816	rBV3	362	204	0.02%	0.002%
89	13.451	3851	3860	3873	rBV2	5648	10114	0.78%	0.097%
90	13.622	3911	3913	3914	rBV	414	210	0.02%	0.002%
91	13.828	3975	3977	3981	rBV3	417	238	0.02%	0.002%
92	13.959	4017	4018	4019	rBV	595	216	0.02%	0.002%
93	14.078	4053	4055	4058	rBV3	652	413	0.03%	0.004%
94	14.210	4094	4096	4100	rBV3	603	413	0.03%	0.004%

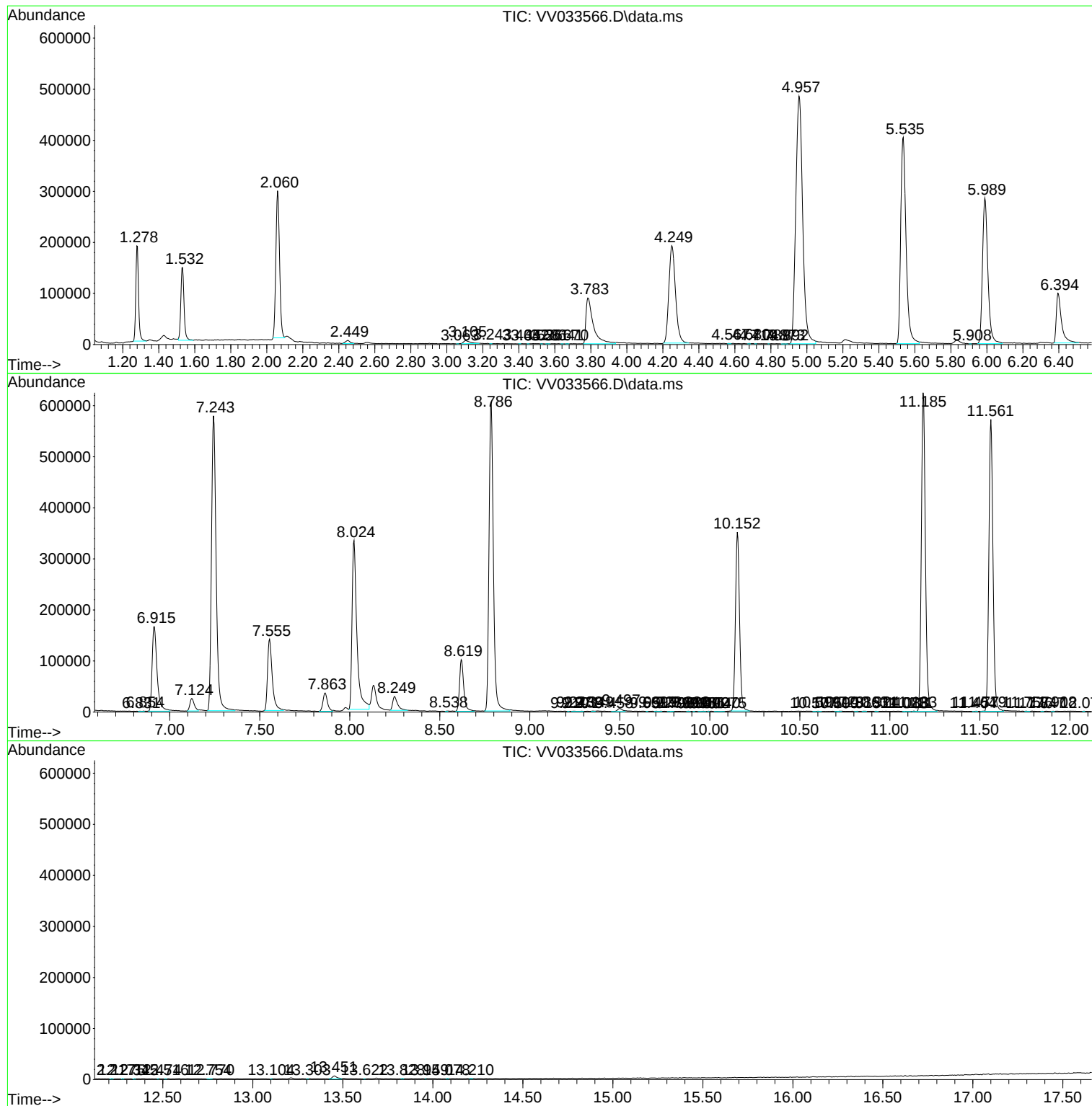
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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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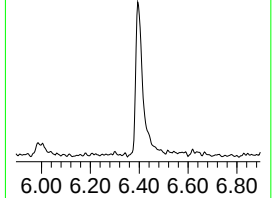
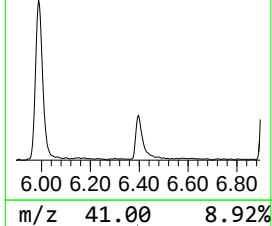
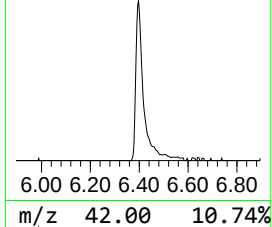
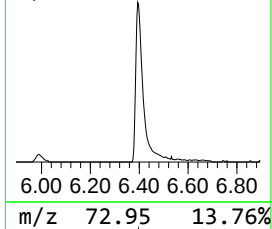
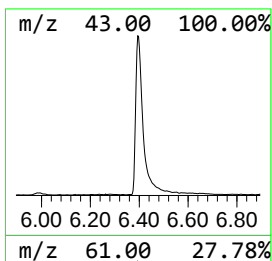
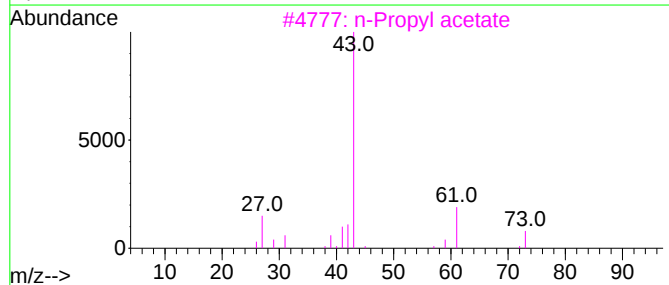
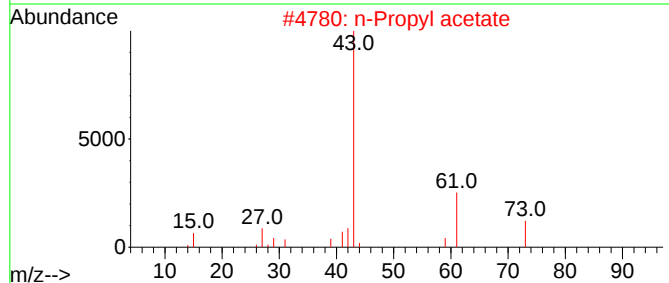
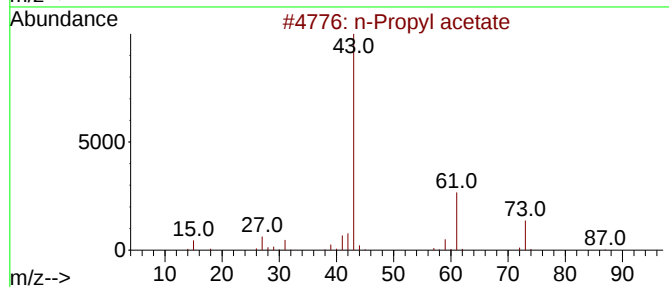
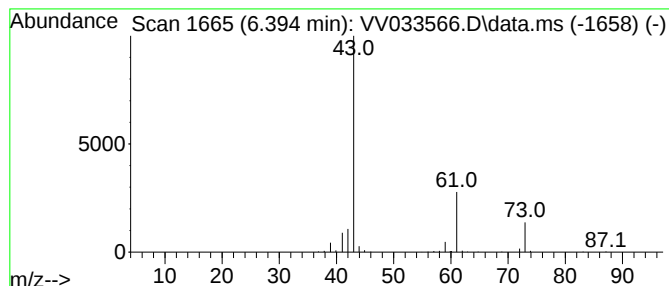
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.394	11.81 ug/L	196428	1,4-Difluorobenzene	5.535

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate			102	C5H10O2	000109-60-4	83
2	n-Propyl acetate			102	C5H10O2	000109-60-4	72
3	n-Propyl acetate			102	C5H10O2	000109-60-4	72
4	n-Propyl acetate			102	C5H10O2	000109-60-4	64
5	n-Propyl acetate			102	C5H10O2	000109-60-4	64



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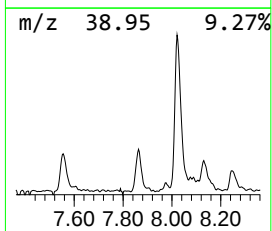
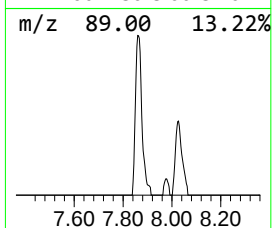
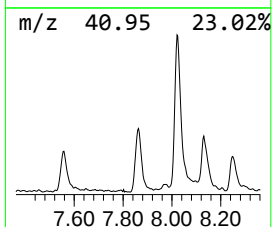
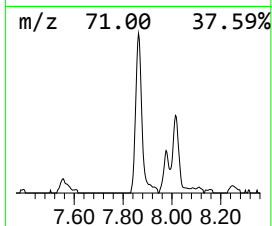
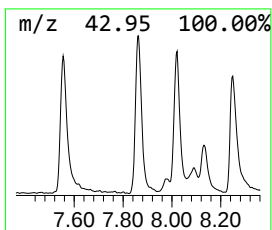
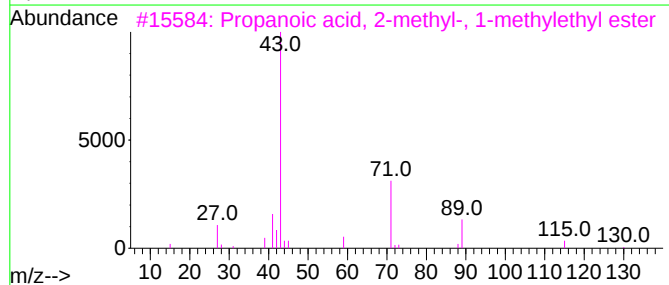
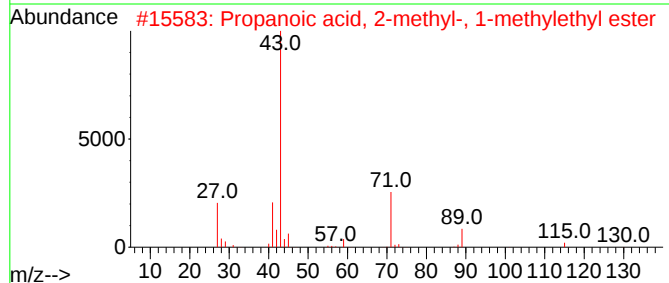
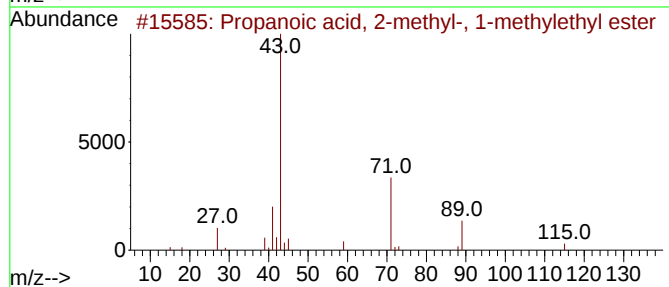
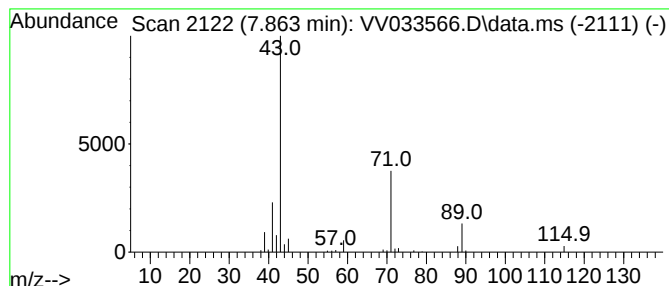
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.863	3.10 ug/L	62666	Chlorobenzene-d5	8.786

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
3			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64



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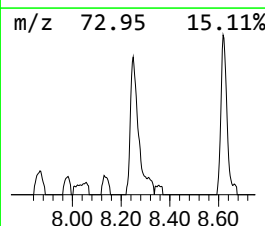
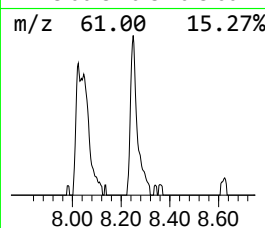
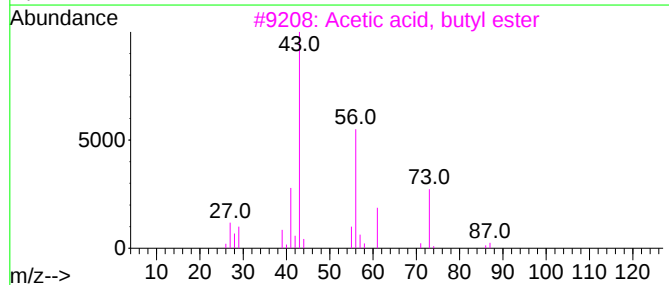
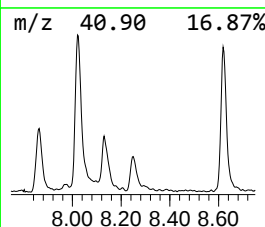
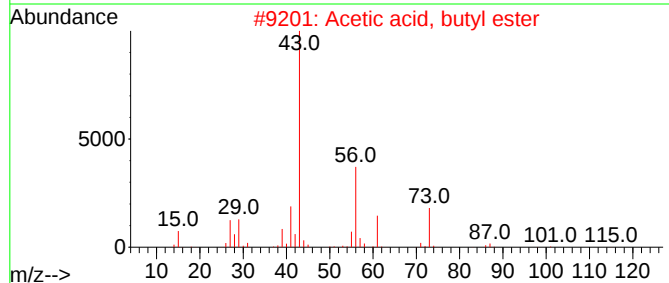
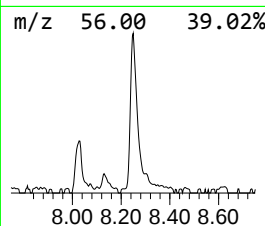
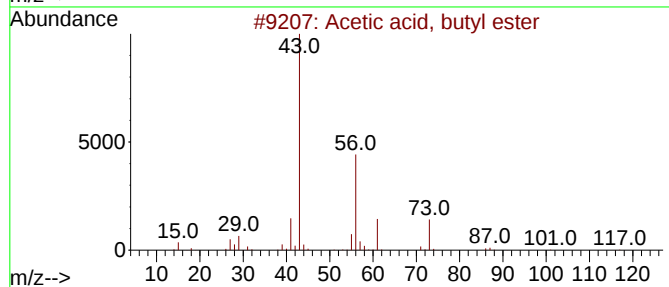
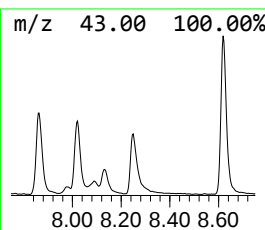
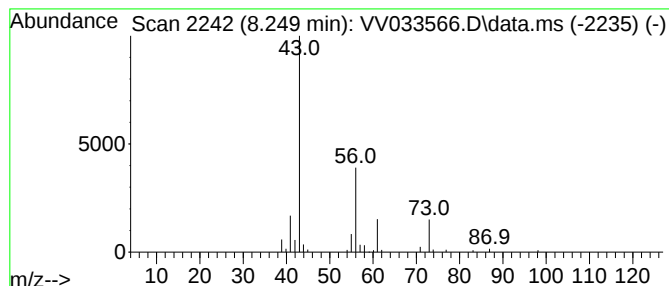
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.249	2.55 ug/L	51582	Chlorobenzene-d5	8.786

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester			116	C6H12O2	000123-86-4	83
2	Acetic acid, butyl ester			116	C6H12O2	000123-86-4	83
3	Acetic acid, butyl ester			116	C6H12O2	000123-86-4	56
4	Acetic acid, butyl ester			116	C6H12O2	000123-86-4	40
5	Acetic acid, hexyl ester			144	C8H16O2	000142-92-7	38



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ClientSampleId :
DCMH4

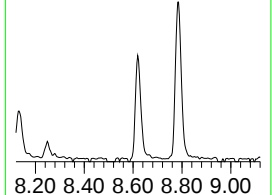
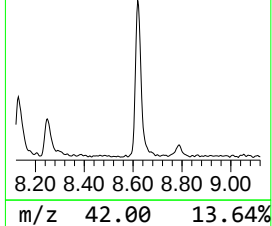
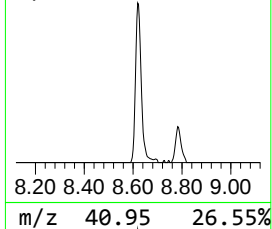
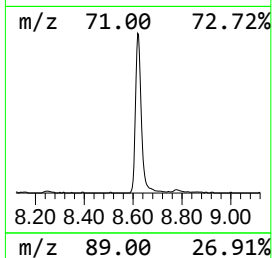
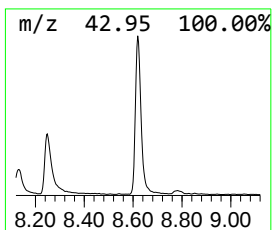
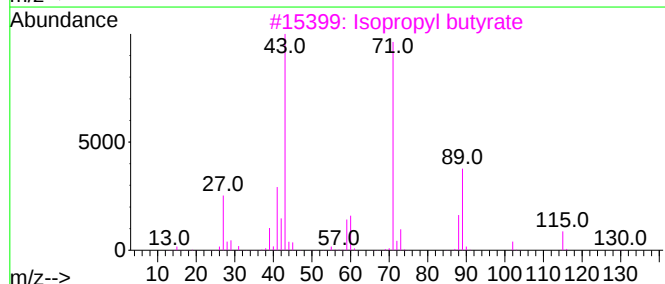
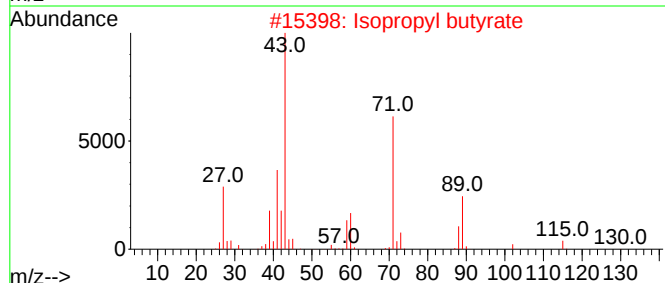
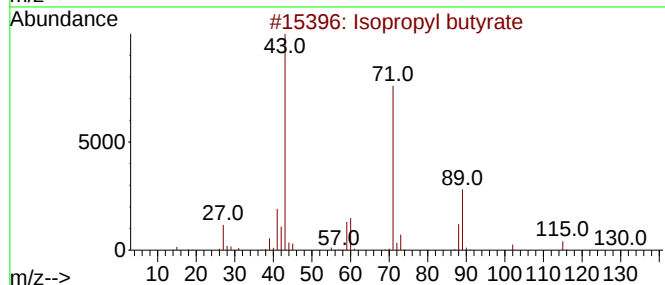
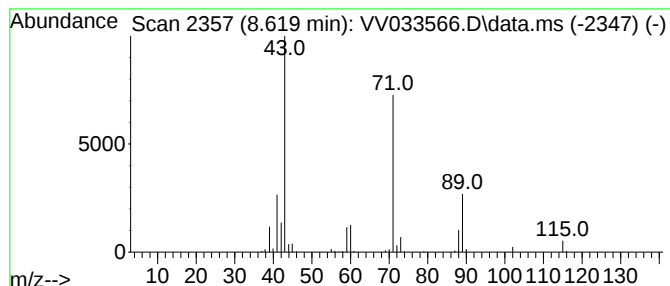
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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.619	8.20 ug/L	165816	Chlorobenzene-d5	8.786

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
2			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	86
4			Isopropyl butyrate	130	C7H14O2	000638-11-9	83
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011024\
Data File : VV033566.D
Acq On : 10 Jan 2024 17:30
Operator : SY/MD
Sample : P1016-04 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCMH4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	6.394	11.8	ug/L	196428	1	5.535	831383	50.0
Propanoic acid,...	7.863	3.1	ug/L	62666	2	8.786	1011310	50.0
Acetic acid, bu...	8.249	2.5	ug/L	51582	2	8.786	1011310	50.0
Isopropyl butyrate	8.619	8.2	ug/L	165816	2	8.786	1011310	50.0